



chain nodes :

21 22 23 24 25 26 27 28 29 30 31 32 34 35 36 37 39 41 42

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

1-42 2-41 6-22 8-27 10-21 14-28 15-19 16-24 16-31 17-25 17-32 19-29 20-23 20-30
21-22 25-26 34-35 35-36 35-37

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 11-13 12-15 13-14 14-15
16-17 16-20 17-18 18-19 19-20

exact/norm bonds :

10-21 11-13 12-15 13-14 14-15 15-19 16-17 16-20 16-24 17-18 18-19 19-20 20-23
34-35 35-36

exact bonds :

1-42 2-41 6-22 8-27 14-28 16-31 17-25 17-32 19-29 20-30 21-22 25-26 35-37

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:I,S03H,C(O)CH3,[*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 39:CLASS 40:Atom 41:CLASS
42:CLASS